
Machine Learning

Topic 3: Instance-based learning (a.k.a. Nearest Neighbor learning)

(with ideas and a few images from Andrew Moore
Check out his site at <http://www.autonlab.org/>)

Classification vs. Regression

- Classification:

Learning a function to map from a n-tuple to a ***discrete*** value from a finite set

- Regression:

Learning a function to map from a n-tuple to a ***continuous*** value

Nearest Neighbor Classifier

- Example of memory-based (a.k.a instance-based, a.k.a case-based) learning
- The basic idea:
 1. Get some example set of cases with known outputs
e.g diagnoses of infectious diseases by experts
 2. When you see a new case, assign its output to be the same as the most similar known case.
Your symptoms most resemble Mr X.
Mr X had the flu.
Ergo you have the flu.

General Learning Task

There is a set of possible examples $X = \{\vec{x}_1, \dots, \vec{x}_n\}$

Each example is an k -tuple of attribute values

$$\vec{x}_1 = \langle a_1, \dots, a_k \rangle$$

There is a target function that maps X onto some finite set Y

$$f : X \rightarrow Y$$

The DATA is a set of tuples $\langle \text{example}, \text{target function values} \rangle$

$$D = \{ \langle \vec{x}_1, f(\vec{x}_1) \rangle, \dots, \langle \vec{x}_m, f(\vec{x}_m) \rangle \}$$

Find a **hypothesis** h such that...

$$\forall \vec{x}, h(\vec{x}) \approx f(\vec{x})$$

Eager vs. Lazy

Eager learning

- Learn model ahead of time from training data
- Explicitly learn h from training data
- E.g. decision tree, linear regression, svm, neural nets, etc.

Lazy learning

- Delay the learning process until a query example must be labeled
- h is implicitly learned from training data
- E.g. Nearest neighbor, kNN, locally weighted regression, etc.

Single Nearest Neighbor

Given some set of training data...

$$D = \{ \langle \vec{x}_1, f(\vec{x}_1) \rangle, \dots, \langle \vec{x}_m, f(\vec{x}_m) \rangle \}$$

...and query point \vec{x}_q , predict $f(\vec{x}_q)$

1. Find the nearest member of the data set to the query

$$\vec{x}_{nn} = \arg \min_{\vec{x} \in D} (d(\vec{x}, \vec{x}_q))$$

distance function
↓

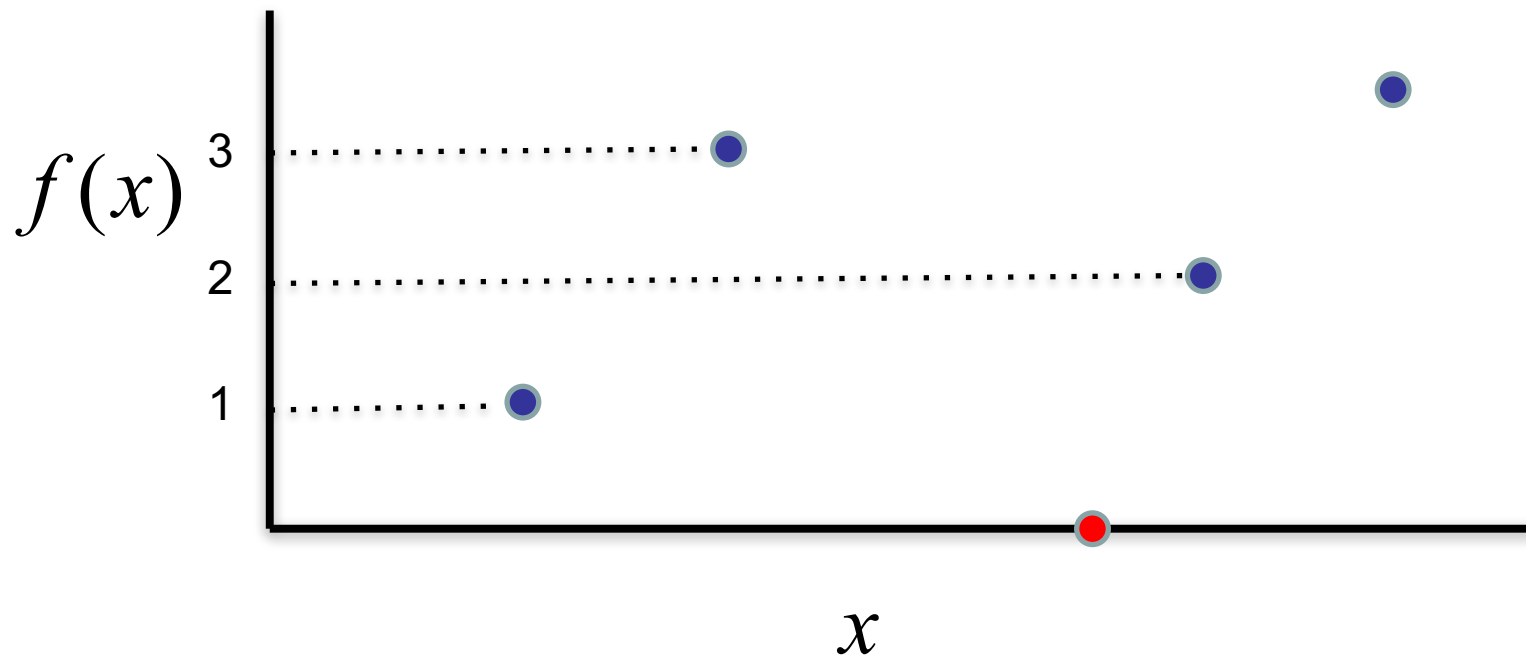
2. Assign the nearest neighbor's output to the query

$$h(\vec{x}_q) = f(\vec{x}_{nn})$$

Our hypothesis
↑

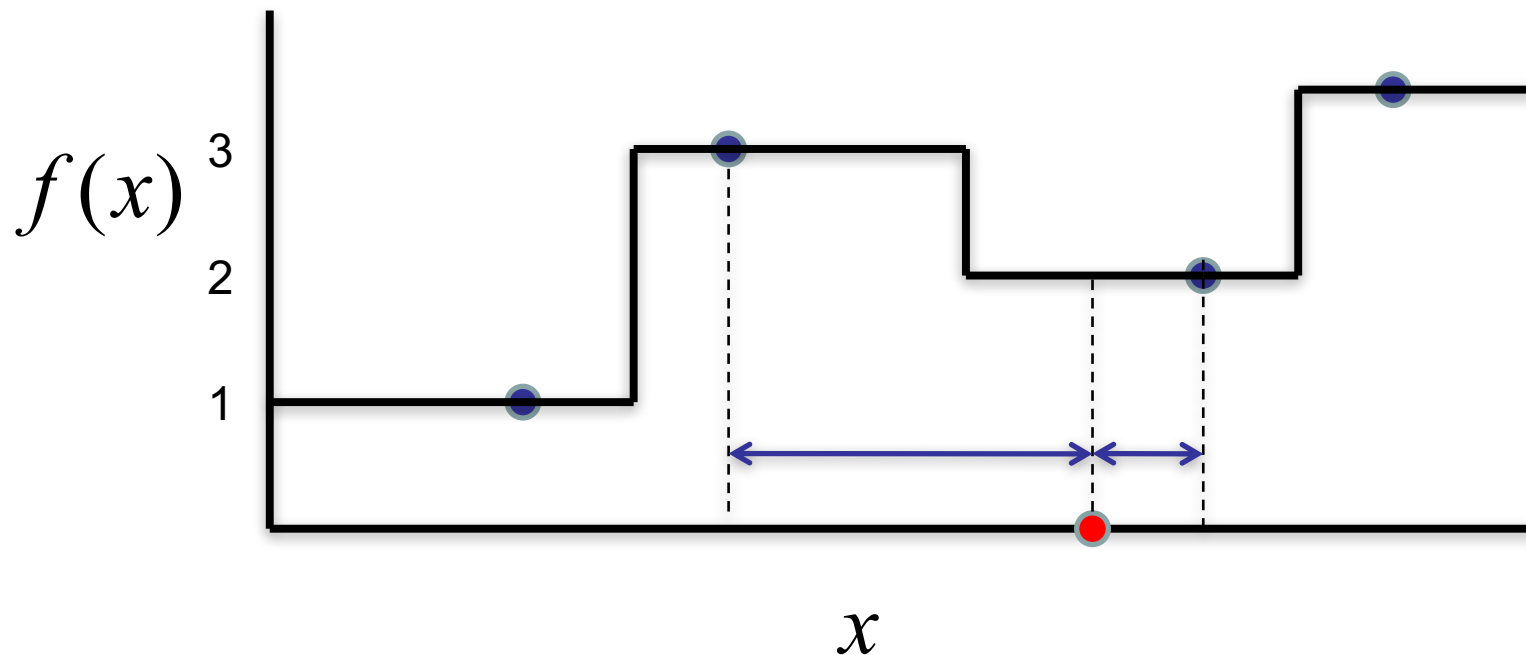
A Univariate Example

- Find closest point. $\vec{x}_{nn} = \arg \min_{x \in D} (d(\vec{x}, \vec{x}_q))$
- Give query its value $f(\vec{x}_q) = f(\vec{x}_{nn})$



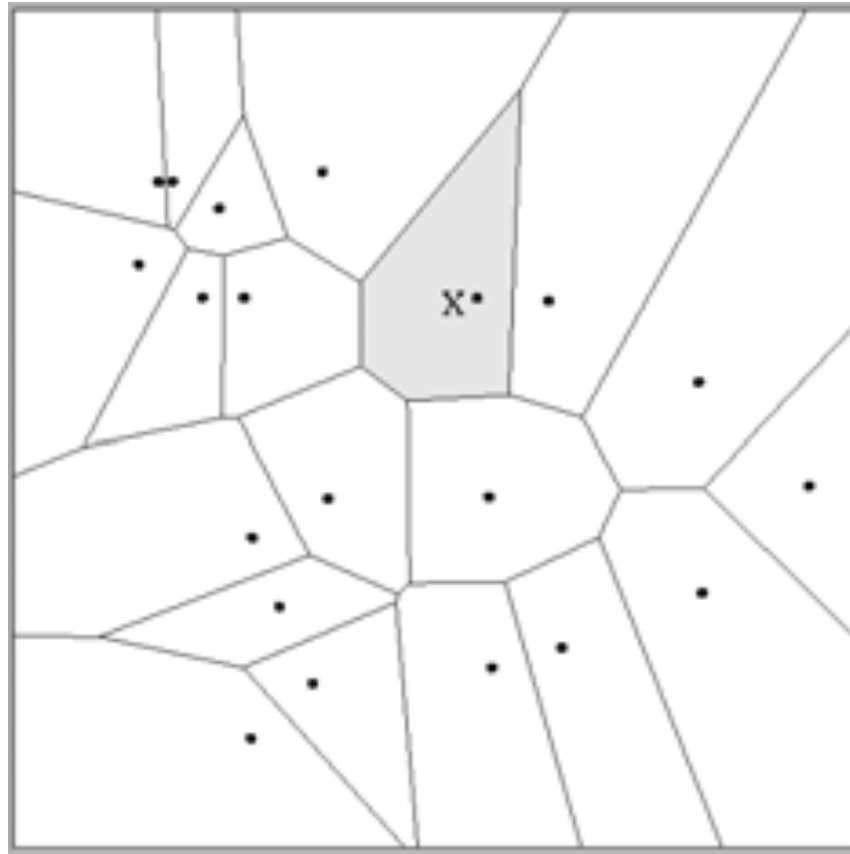
A Univariate Example

- Find closest point. $\vec{x}_{nn} = \arg \min_{x \in D} (d(\vec{x}, \vec{x}_q))$
- Give query its value $f(\vec{x}_q) = f(\vec{x}_{nn})$



A Two-dimensional Example

- Voronoi diagram



What makes a memory based learner?

- A distance measure
Nearest neighbor: typically Euclidean
- Number of neighbors to consider
Nearest neighbor: One
- A weighting function (optional)
Nearest neighbor: unused (equal weights)
- How to fit with the neighbors
Nearest neighbor: Same output as nearest neighbor

K-nearest neighbor

- A distance measure
Euclidean
- Number of neighbors to consider
K
- A weighting function (optional)
Unused (i.e. equal weights)
- How to fit with the neighbors
regression: average output among K nearest neighbors.
classification: most popular output among K nearest neighbors

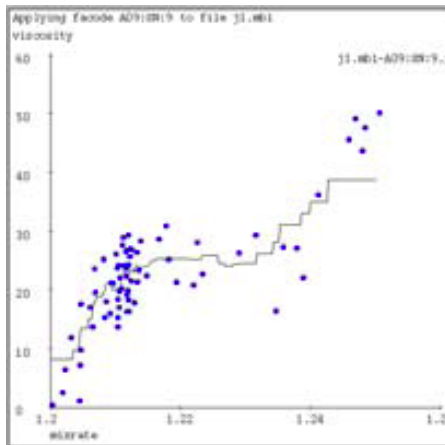
Choosing K

- Too small of K fits the output to the noise in the dataset (overfit)
- Too large of K can make decision boundaries in classification indistinct (underfit)
- Choose K empirically using cross-validation

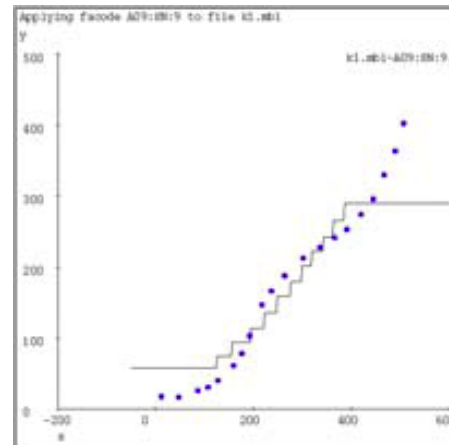
Ex. of KNN for classification

<http://demonstrations.wolfram.com/KNearestNeighborKNNClassifier/>

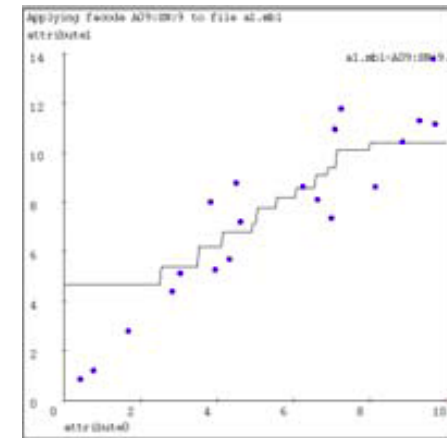
Ex. Of kNN regression where $K=9$



Reasonable job
Did smooth noise



Screws up on the ends



OK, but problem on
the ends again.

Kernel Regression

- A distance measure: *Scaled Euclidean*
- Number of neighbors to consider: *All of them*
- A weighting function:

$$w_i = \exp\left(\frac{-d(x_i, x_q)^2}{K_w^2}\right)$$

Nearby points to the query are weighted strongly, far points weakly. The K_w parameter is the Kernel Width.

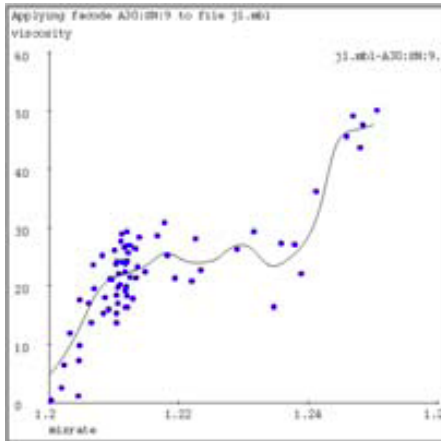
- How to fit with the neighbors:

$$h(x_q) = \frac{\sum_i w_i \cdot f(x_i)}{\sum_i w_i}$$

A weighted average

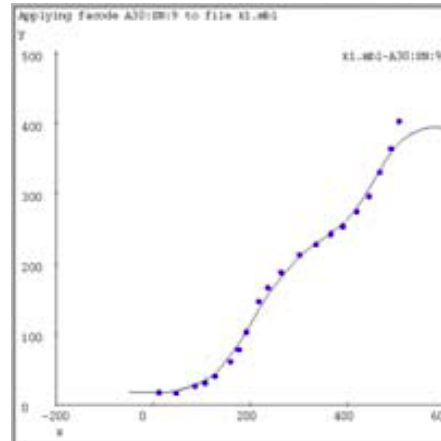
Kernel Regression

Kernel Weight = $1/32$
of X-axis width



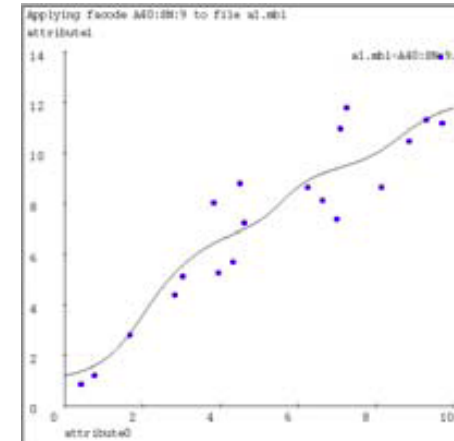
A better fit than KNN?

Kernel Weight = $1/32$
of X-axis width



Definitely better than
KNN! Catch: Had to play
with kernel width to get
This result

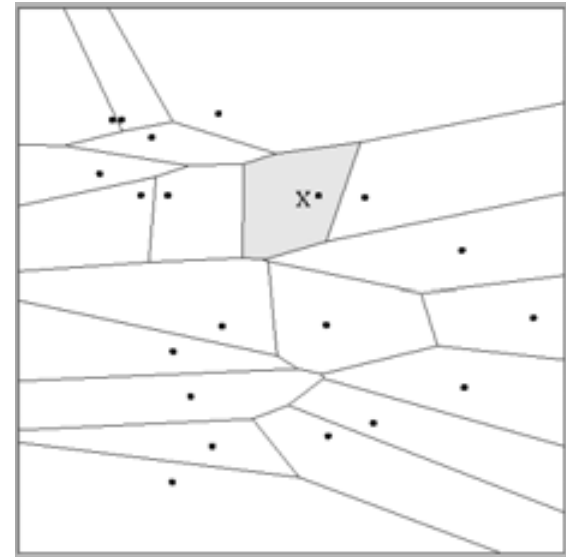
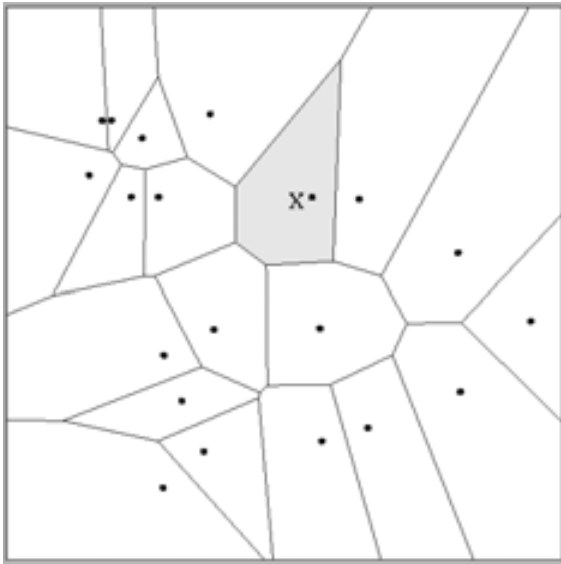
Kernel Weight = $1/16$
of X-axis width



Nice and smooth, but
are the bumps
justified, or is this
overfitting?

Weighting dimensions

- Suppose data points are two-dimensional
- Different dimensional weightings affect region shapes



$$d(x, y) = (x_1 - y_1)^2 + (x_2 - y_2)^2 \quad d(x, y) = (x_1 - y_1)^2 + (3x_2 - 3y_2)^2$$

kNN and Kernel Regression

Pros

- Robust to noise
- Very effective when training data is sufficient
- Customized to each query
- Easily adapts when new training data is added

Cons

- How to weight different dimensions?
- Irrelevant dimensions
- Computationally expensive to label a new query
- High space requirements (must retain each training example)

Locally Weighted (Linear) Regression

- Linear regression: global, linear

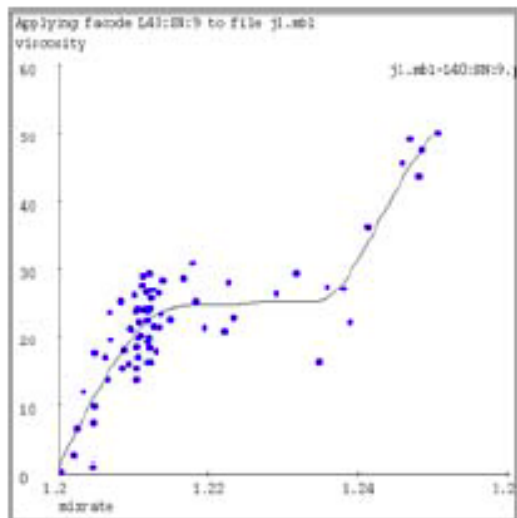
$$Err = \sum_{\vec{x} \in D} \frac{1}{2} (f(\vec{x}) - h(\vec{x}))^2 \quad h(\vec{x}) = \vec{a}^T \vec{x} + \vec{b}$$

- kNN: local, constant
- LWR: local, linear

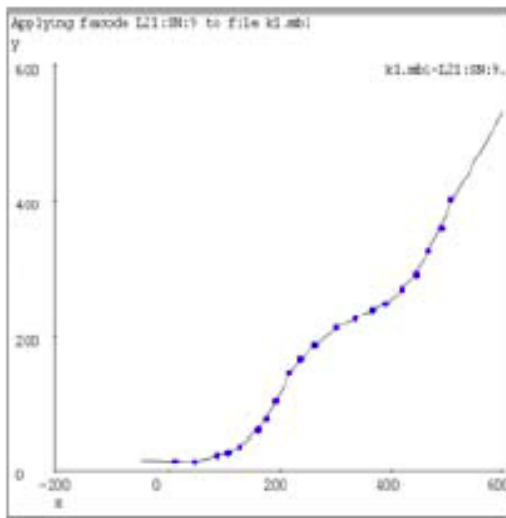
$$\vec{x}_{nn} = \arg \min_{\vec{x} \in D} (d(\vec{x}, \vec{x}_q))$$

$$Err(x_q) = \sum_{x \in D} \frac{1}{2} (f(x) - h(x))^2 \exp\left(\frac{-d(x, x_q)^2}{K_w^2}\right)$$

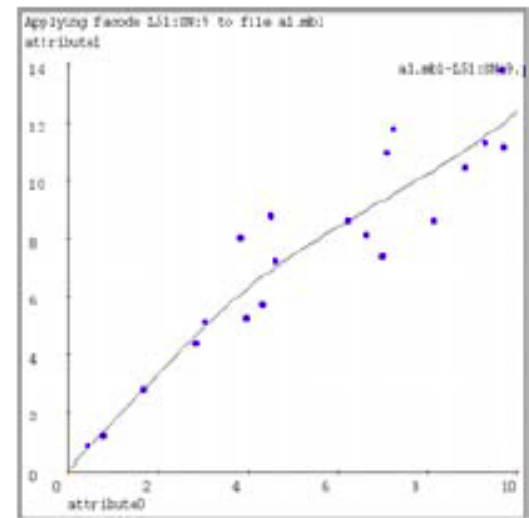
Locally Weighted (Linear) Regression



KW = 1/16 of x-axis width.



KW = 1/32 of x-axis width.

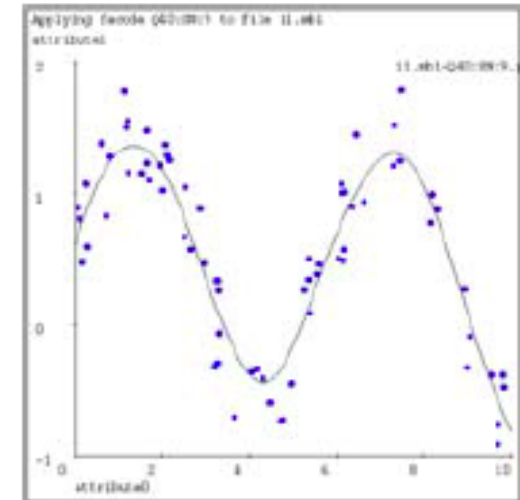
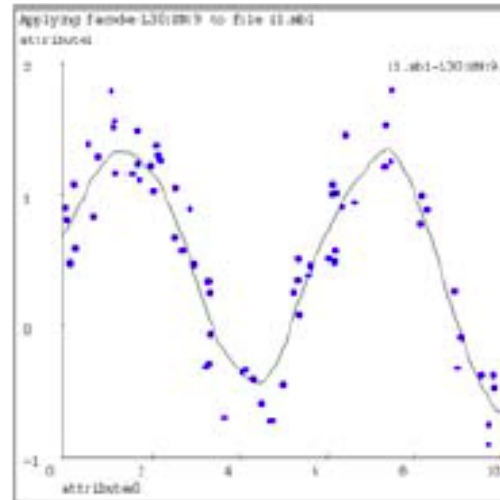
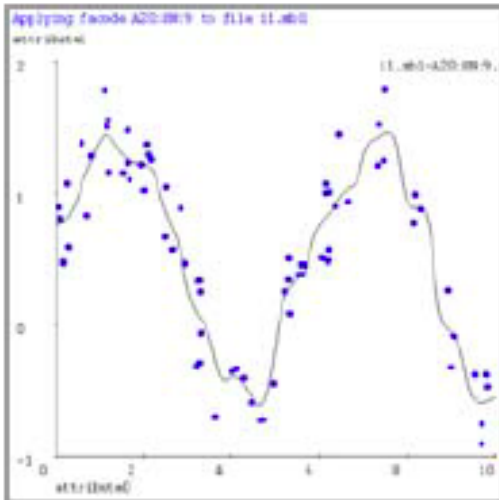


KW = 1/8 of x-axis width.

Nicer and smoother, but even now, are the bumps justified, or is this overfitting?

Locally Weighted Polynomial Regression

- Use a polynomial instead of a linear function to fit the data locally
 - Quadratic, cubic, etc.



$KW = 1/100$ x-axis

$KW = 1/40$ x-axis

$KW = 1/15$ x-axis

Memory-based Learning

Pros

- Easily adapts to new training examples (no-retraining required)
- Can handle complex decision boundaries and functions by considering the query instance when deciding how to generalize

Cons

- Requires retaining all training examples in memory
- Slow to evaluate a new query
- Evaluation time grows with the dataset size

Summary

- Memory-based learning are “lazy”
 - Delay learning until receiving a query
- Local
 - Training data that is localized around the query contribute more to the prediction value
- Non-parametric
- Robust to noise
- Curse of dimensionality
 - Irrelevant dimensions
 - How to scale dimensions

Summary

- Nearest neighbor
 - Output the nearest neighbor's label
- kNN
 - Output the average of the k NN's labels
- Kernel regression
 - Output weighted average of all training data's (or k NN's) labels
- Locally weighted (linear) regression
 - Fit a linear function locally